EQUILIBRIUM FLUCTUATIONS IN MEAN-FIELD DISORDERED MODELS [8]

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Introduction

Equilibrium Measure as Large Deviation

Consider a system of size N at thermal equilibrium. The probability of observing $o = O/N$ away from its average,

$$P(o) \propto e^{-Nf(o)} ,$$

where $f(o)$ is the large deviation function related to this probability, i.e., the intensive free energy of the system. Its global minimum, o^*, corresponds to the average observed, $\langle o\rangle = o^*$, in the thermodynamic limit $N \to \infty$. Given $f(o)$, the variance of fluctuations around o^* is:

$$\langle o^2\rangle - \langle o\rangle^2 = \frac{1}{N\partial_o^2 f(o)|_{o=o^*}} .$$

For large enough N, the probability $P(o)$ can be approximated by a Gaussian distribution of this variance.

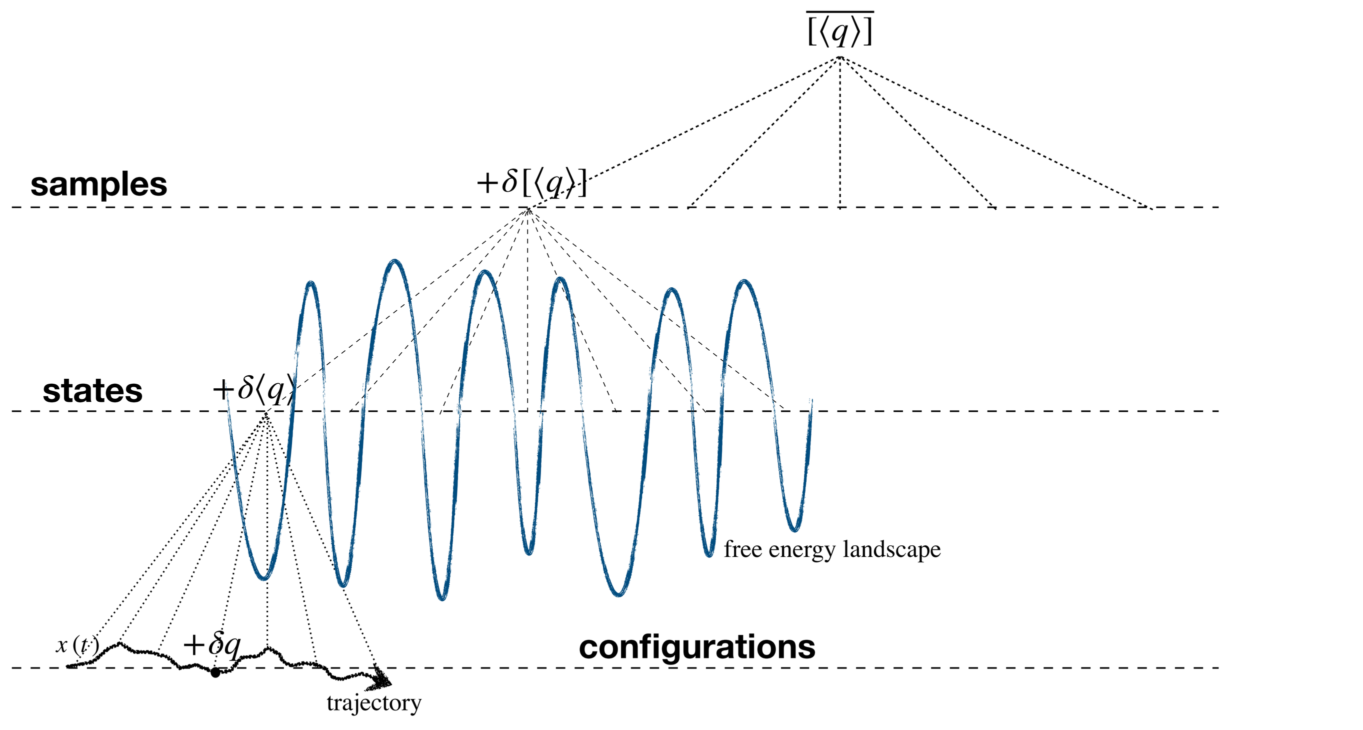
Small Fluctuations

- ***intra-state*** **fluctuations** δq: equilibrium exploration of a state;
- ***inter-state*** **fluctuations** $\delta\langle q\rangle$: variability of states in a given system;
- ***sample-to-sample*** **fluctuations** $\delta[\langle q\rangle]$: variability between different samples (disorders).

Susceptibilities [1,2]

In the *small-fluctuation* regime, each level of the hierarchy exhibits Gaussian fluctuations. Three susceptibilities (or variances) proportional to $1/N$:

$$\chi_{\rm intra} = \overline{[\langle \delta q \delta q\rangle]}$$
$$\chi_{\rm inter} = \overline{[\delta\langle q\rangle \delta\langle q\rangle]}$$
$$\chi_{\rm dis} = \overline{\delta[\langle q\rangle]\delta[\langle q\rangle]}$$



$\langle\bullet\rangle$, thermal average in a state, $[\bullet]$, average over states of a sample, $\overline{\bullet}$, average over different samples.

Methods

Replica Method and Mass Matrix [2,3]

The average over the quenched disorder is evaluated by the replica method. The replicated free energy $F(\mathbb{Q})$ is a large deviation function for the $n \times n$ overlap matrix $\mathbb{Q}^n$,

$$P(\mathbb{Q}) \propto e^{-NF(\mathbb{Q})},$$

each element $\mathbb{Q}_{a,b} = x_a \cdot x_b/N$, for a scalar product $\cdot$ in the space of configurations x. In the thermodynamic limit, at fixed n, the measure concentrates on the most probable matrix:

$$\mathbb{Q}^*{}_{a,b} = \overline{[\langle q_{ab}\rangle]} = \overline{[\langle x_a \cdot x_b\rangle]}/N.$$

In this context, fluctuations are obtained from the Hessian (or mass matrix) of $F(\mathbb{Q})$ around the saddle point $\mathbb{Q}^*$,

$$\mathbb{M}_{ab;cd} \equiv \partial_{q_{ab}}\partial_{q_{cd}} F(\mathbb{Q})|_{\mathbb{Q}=\mathbb{Q}^*} .$$

The inverse $\mathbb{G}_{ab;cd} = (\mathbb{M}^{-1})_{ab;cd}$ of the mass matrix encodes overlap fluctuations in the *small-fluctuation* regime,

$$\overline{[\langle q_{ab} q_{cd}\rangle]} - \overline{[\langle q_{ab}\rangle][\langle q_{cd}\rangle]} = \frac{1}{N}\mathbb{G}_{ab;cd} ,$$

Given a replica symmetric ansatz, the mass matrix (RSMM) reads:

$$\mathbb{M}^{\rm RS}_{ab;cd} = \frac{m_1}{2}(\delta_{ac}\delta_{bd}+\delta_{ad}\delta_{bc})+\frac{m_2}{4}(\delta_{ac}+\delta_{ad}+\delta_{bc}+\delta_{bd})+m_3$$

which depends on the three parameters m_1, m_2, m_3.

Estimating Equilibrium Fluctuations [3,8]

Given the two-time correlation $C(t,t')$ inside a state ^{0}, we evaluate it at equidistant point in time (s.t. the system as typically relaxed within a state), and obtain the matrix of correlations $C_{i,j}$. There are two different ways of evaluating the variance of *intra-state* fluctuations,

$$N^{-1}\hat\chi^0_{\rm th} \approx {\rm Mean}_i[{\rm Var}_j[C^0_{i,j}]] ,$$
$$N^{-1}\hat\chi^0_{\rm dyn} \approx {\rm Var}_{i,j}[C^0_{i,j}] ,$$

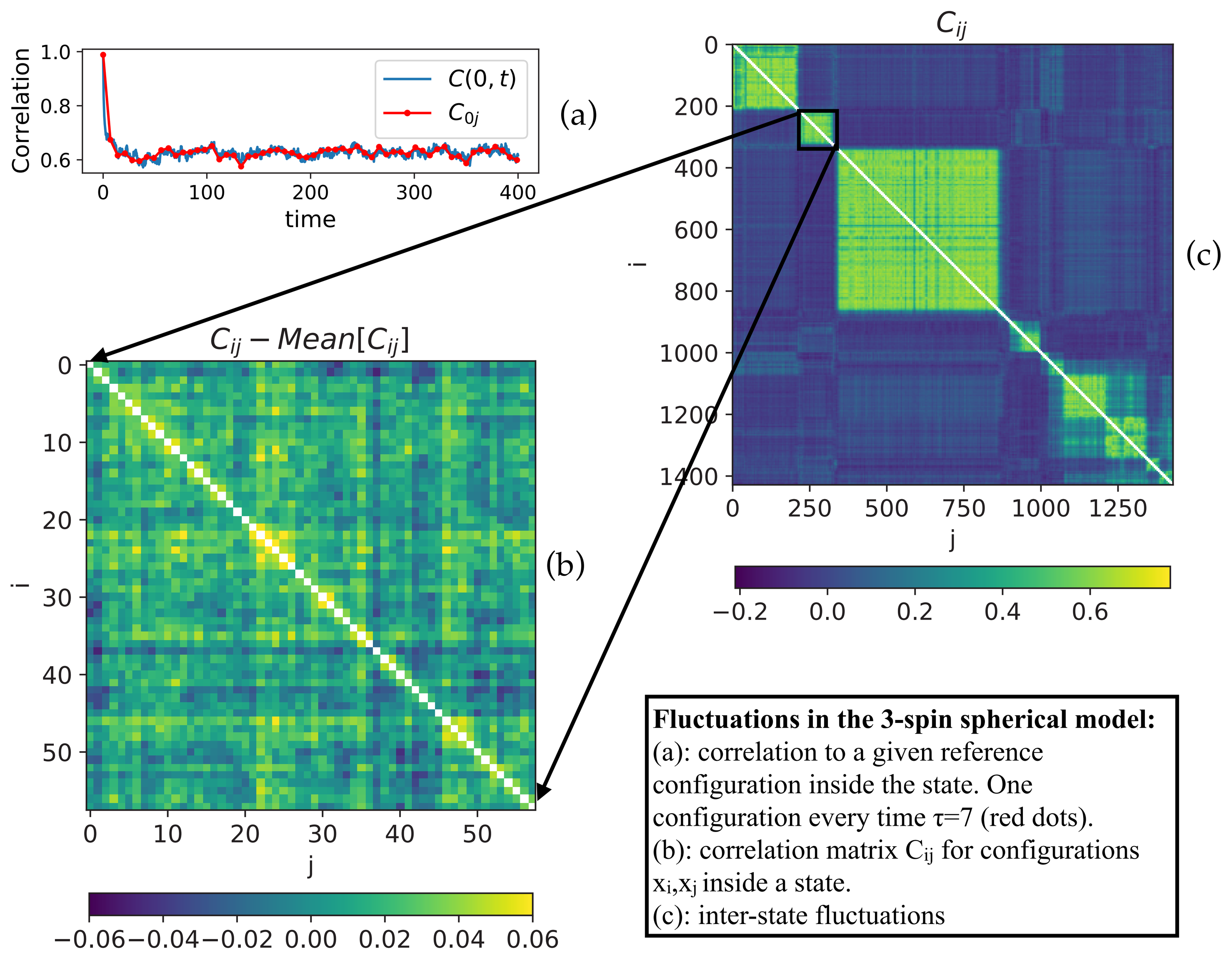
s.t. $\hat\chi^0_{\rm th} < \hat\chi^0_{\rm dyn}$. Complementary to these, there are two *sample-to-sample* susceptibilities (i.e. $\chi_{\rm inter}+\chi_{\rm dis}$):

$$N^{-1}\hat\chi_{\rm het} \approx {\rm Var}_{k,i}[{\rm Mean}_j[C^k_{i,j}]] ,$$
$$N^{-1}\hat\chi_{\rm var} \approx {\rm Var}_k[{\rm Mean}_{i,j}[C^k_{i,j}]]$$

From Mass Matrix to Susceptibilities [2,8]

Susceptibilities can be written in terms of m_1, m_2, m_3.

Intra-state	
$\hat\chi^0_{\rm th}(m_1,m_2)$	$\hat\chi^0_{\rm dyn}(m_1,m_2)$
Sample-to-sample	
$\hat\chi_{\rm het}(m_1,m_2,m_3)$	$\hat\chi_{\rm var}(m_1,m_2,m_3)$
Total	
$\chi_{\rm tot} = \hat\chi_{\rm het} + \overline{[\hat\chi^0]}_{\rm th} = \hat\chi_{\rm var} + \overline{[\hat\chi^0]}_{\rm dyn}$	



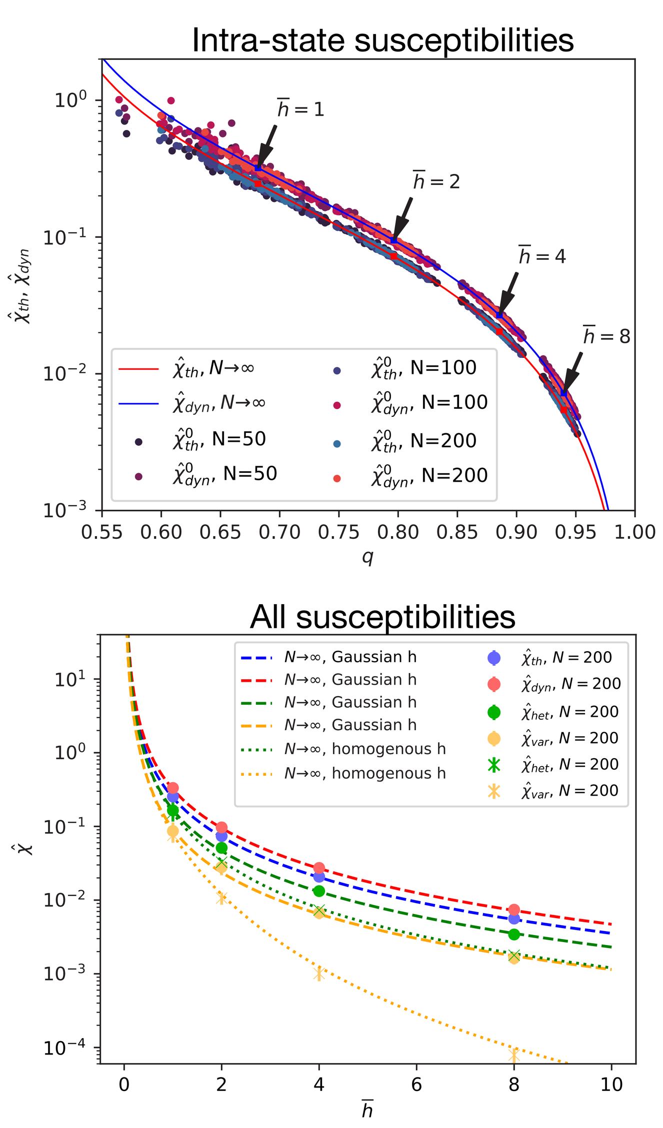
Fluctuations in the 3-spin spherical model:
(a): correlation to a given reference configuration inside the state. One configuration every time τ=7 (red dots).
(b): correlation matrix C_{ij} for configurations x_i, x_j inside a state.
(c): inter-state fluctuations

Simulations

2-spin Spherical with External Field [4,8]

$$H = -\sum_{ij}^N J_{ij}s_i s_j - \sum_i h_i s_i$$

$\sum_i^N s_i^2 = N$, J_{ij}, Gaussian J_{ij} of variance $\frac{1}{2}N/\binom{N}{p}$, and Gaussian h_i of variance $\bar h^2$.

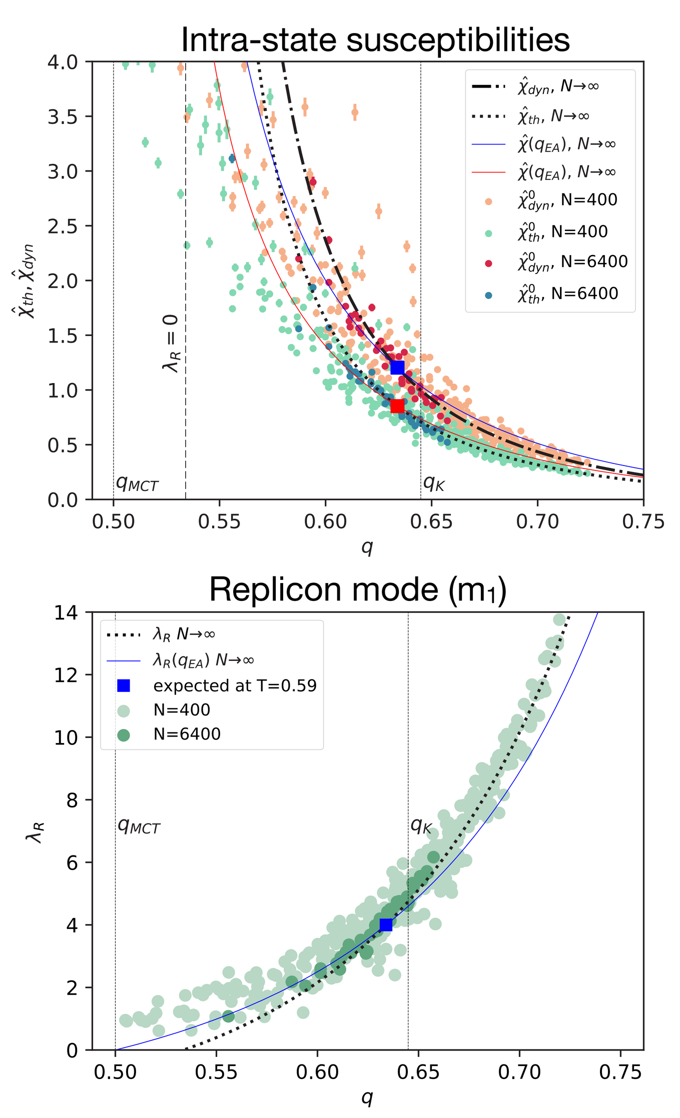


RFOT

3-spin Spherical [5,8]

$$H = -\sum_{ijk}^N J_{ijk}s_i s_j s_k$$

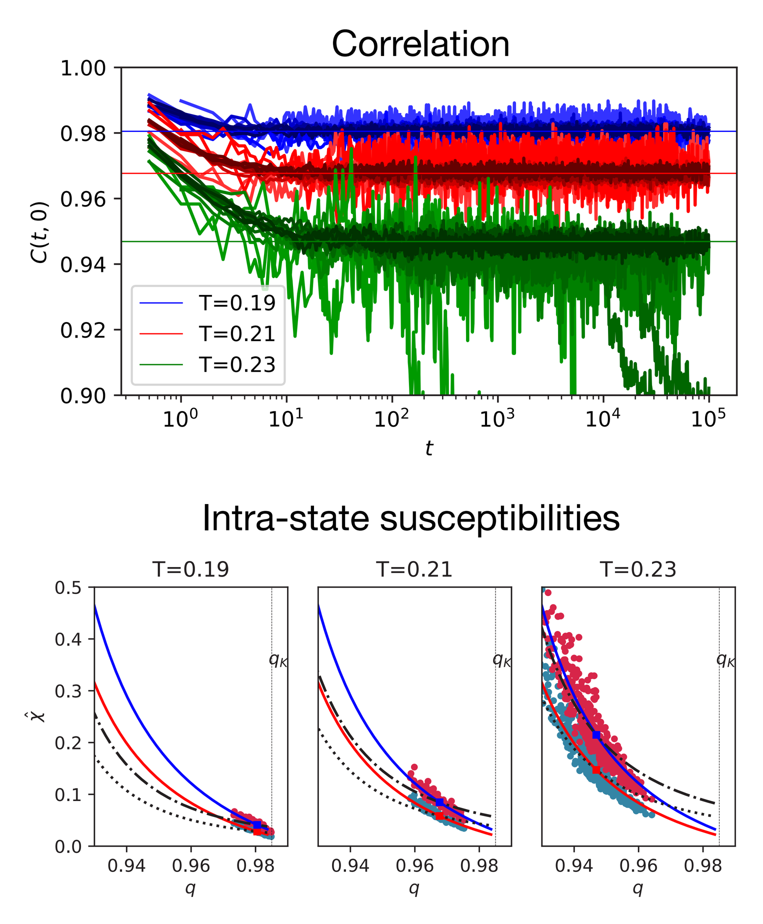
$\sum_i^N s_i^2 = N$ and Gaussian J_{ij} of variance $\frac{1}{2}N/\binom{N}{p}$.
The dynamical transition is at $T_{\rm MCT} \approx 0.6124$.



Random Orthogonal Model [6,8]

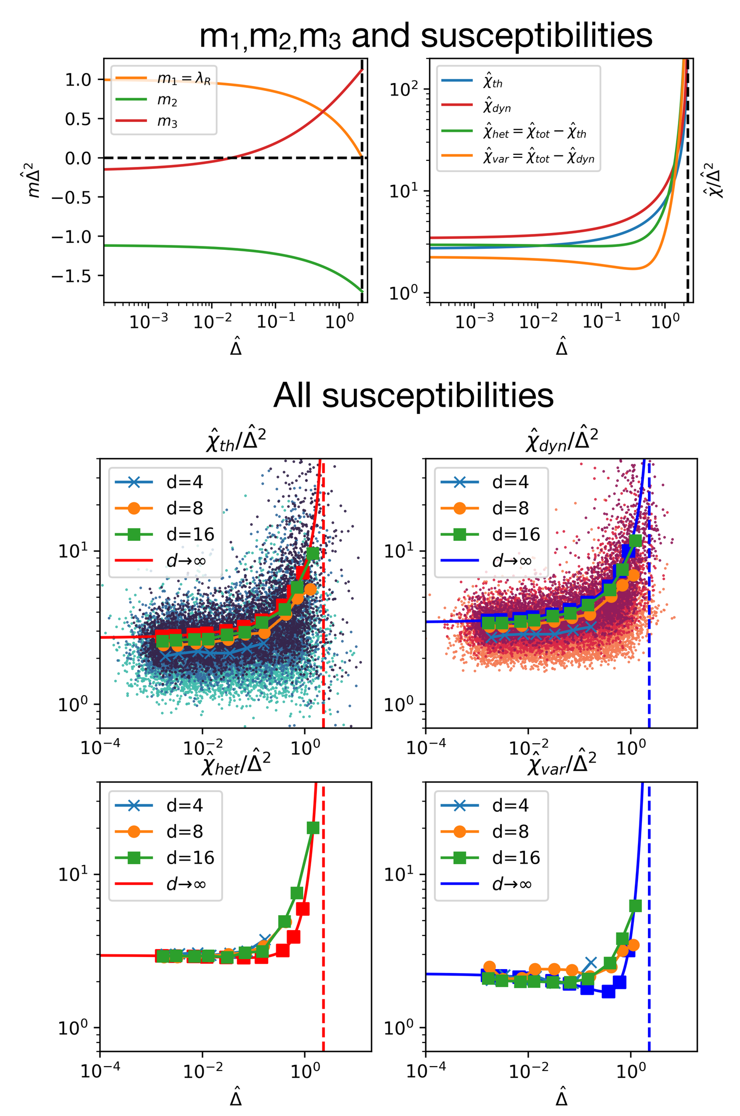
$$H = \sum_{ij} J_{ij}s_i s_j , \qquad J_{ij} = [O^T D O]_{ij}$$

Ising spins, $s_i = \pm 1$, O is a random orthogonal matrix and D is a diagonal matrix of elements iid from a pdf $P(d)$. We chose $P(d) = \alpha\delta(d-1) + (1-\alpha)\delta(d+1)$, with $\alpha = 0.3$, which gives a RFOT phenomenology. $T_{\rm MCT} \approx 0.2465$.



Random Lorentz Gas [7,8]

A tracer particle is at equilibrium within a sea of hard spherical particles in d dimensions. The scaled density $\hat\varphi = 2^d\varphi/d$ is fixed. Simulation are performed at $\hat\varphi = 2.7, 3, 3.5, 5, 7, 10, 15, 20, 30, 40$. The dynamical transition is at $\hat\varphi_d \approx 2.4$.



Perspectives

Following the approach developed in Ref. [2] we have derived explicit formulas connecting the replica symmetric mass matrix and two different kinds of susceptibilities, sample-to-sample and intra-state fluctuations. The results perfectly describe $1/N$ (or $1/d$) fluctuations of the overlaps around their thermodynamic value in the case of disordered model belonging to the standard RS class and to the RFOT class. Reverse-engineering the process, one could imagine having a disordered system at equilibrium for which the Hamiltonian is not known but can be described by building a local RS free energy potential that capture its small fluctuations in the thermodynamic limit. Following the numerical approach presented here, it is possible to derive from the two intra-state susceptibilities $\chi_{\rm th}, \chi_{\rm dyn}$ the relative m_1 and m_2 of each state and from the sample-to-sample susceptibility $\chi_{\rm het}$ the third parameter m_3. One can therefore build the mass matrix, which is then the Gaussian overlap action (effective potential) that describes the equilibrium fluctuations of this system.

References

[1] L. Berthier and R. L. Jack, Phys. Rev. E 76, 041509 (2007).
[2] S. Franz, G. Parisi, F. Ricci-Tersenghi, and T. Rizzo, Eur. Phys. J. E 34, 102 (2011).
[3] S. Franz, H. Jacquin, G. Parisi, P. Urbani, and F. Zamponi, J. Chem. Phys. 138, 12A540 (2013).
[4] J. Baik, E. Collins-Woodfin, P. Le Doussal, and H. Wu, J. Stat. Phys. 183, 31 (2021)
[5] G. Folena, S. Franz and F. Ricci-Tersenghi, J. Stat. Mech. (2021)
[6] R. Cherrier, D. S. Dean, and A. Lefevre, Phys. Rev. E 67 (2003)
[7] G. Biroli, P. Charbonneau, G. Folena, Yi Hu, and F. Zamponi, arXiv:2109.11822 (2021)

[8] arXiv:2202.07560